

# Molecular Line and Continuum Opacities for Modeling of Extrasolar Giant Planet and Cool Stellar Atmospheres

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## Abstract

The molecular line and continuum opacities are investigated in the atmospheres of cool stars and Extrasolar Giant Planets (EGPs). Using a combination of *ab initio* and experimentally derived potential curves and dipole transition moments, accurate data have been calculated for rovibrationally-resolved oscillator strengths and photodissociation cross sections in the  $B' \ ^2\Sigma^+ \leftarrow X \ ^2\Sigma^+$  and  $A \ ^2\Pi \leftarrow X \ ^2\Sigma^+$  band systems in MgH. We also report our progress on the study of the electronic structure of LiCl and FeH.

## 1. Introduction

The lack of accurate and complete molecular line and continuum opacity data has been a serious limitation to developing atmospheric models of cool stars and Extrasolar Giant Planets (EGPs). In fact, sophisticated modeling programs, such as the PHOENIX code (Hauschildt & Baron, 1999), require high quality opacity data in order to produce synthetic spectra and predict physical parameters (surface chemical composition, effective temperature, etc). Typically, atmosphere models include molecular bands with hundreds of millions of spectral lines, mostly derived from molecular band models. Moreover, few models consider the effect of molecular photodissociation processes which may play a role in the opacity at visible and UV wavelengths. In this work, we report our progress on the calculations of line and continuum opacities resulting from the presence of three molecules, MgH (Skory *et al.* 2002; Weck, Stancil, & Kirby 2002a; Weck *et al.* 2002b,c), LiCl and FeH.

## 2. Magnesium hydride

Accurate SDTCI potential-energy surfaces calculated by Saxon, Kirby & Liu (1978) have been used for the  $B' \ ^2\Sigma^+$ ,  $A \ ^2\Pi$  and  $X \ ^2\Sigma^+$  electronic states of  $^{24}\text{MgH}$ , together with their connecting transition dipole moments, over the range  $R = 2.2 a_0$  to  $9.5 a_0$ . For both the short- and long-range interactions, they have been extrapolated by an exponential fit. In Figure 1, the product of the rotational oscillator strengths  $f_{v',J',v'',J''}$  and the degeneracy factor  $g_{J',J''}$  as a function of the absorbed photon energy is shown for the A-X bound-bound transitions. Our calculated spectrum appears to be more compact than the results of Kurucz (1993) obtained by extrapolation. In particular, the differences observed on the wavelength range

19000 – 20500  $\text{cm}^{-1}$  may have significant consequences for high temperature studies (e.g., non-equilibrium chemistry models of M and L dwarf atmospheres). For the  $B' - X$  bound-bound transitions, a good qualitative and quantitative agreement is observed with the results of Kurucz (1993).

The LTE rovibrationally-resolved photodissociation cross sections  $\sigma_{v'',J''}$  for the A-X transitions are presented in Figure 2 as functions of wavelength and temperature (Boltzmann distribution). Rotational cross sections are characterized by shape resonances arising from rotational predissociation of quasi-bound levels of the  $A^2\Pi$  electronic state near threshold. The cross section from the ground RV level,  $v'' = 0, J'' = 0$ , is also represented for photodissociation through the  $B'-X$  transitions.

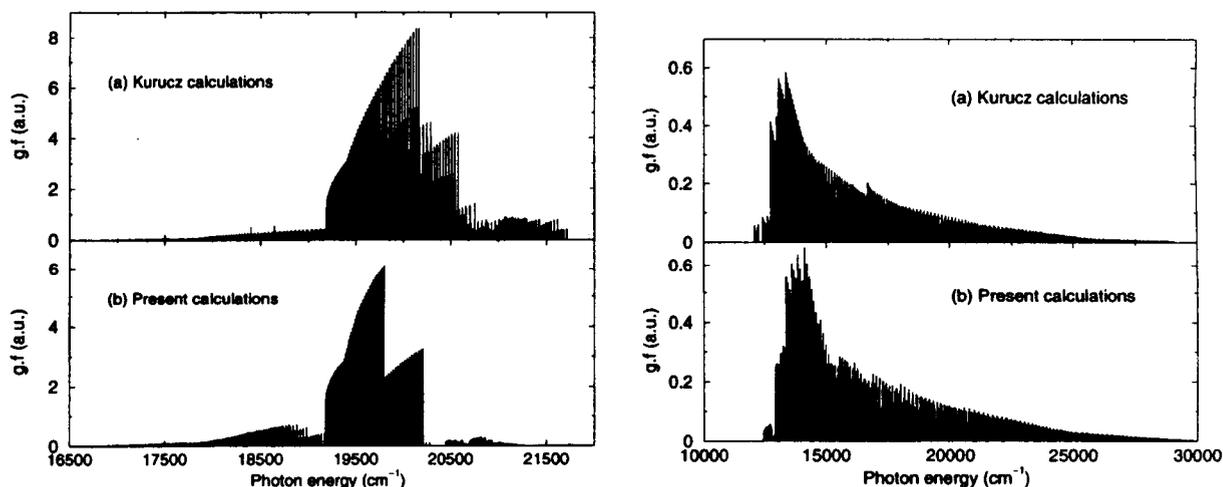


Fig. 1.— Product of the rotational oscillator strengths  $f_{v'',J'',v'',J''}$  and the degeneracy factor  $g_{J'',J''}$  as a function of the absorbed photon energy. Left:  $A \leftarrow X$  transitions; right:  $B' \leftarrow X$  transitions.

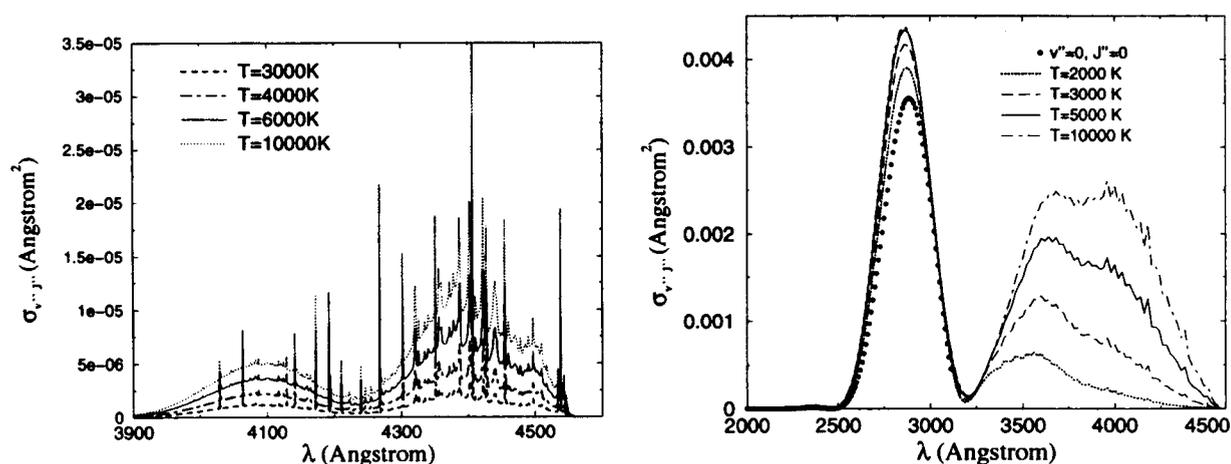


Fig. 2.— LTE photodissociation cross sections  $\sigma_{v'',J''}$  as functions of wavelength and temperature (Boltzmann distribution). Left:  $A \leftarrow X$  transitions; right:  $B' \leftarrow X$  transitions.

### 3. Lithium Chloride and Iron Hydride

From our *ab initio* SDCI calculations using the ALCHEMY code (Mc Lean *et al.* 1991), we have obtained five  $^1\Sigma$  and five  $^1\Pi$  electronic states, thus giving four additional electronic states than that calculated with a valence-bond method by Zeiri & Balint-Kurti (1983). Calculations to obtain the energy surfaces over a large internuclear distance range are underway. Calculations have been performed using the coupled cluster method (CCSD(T)) near the equilibrium distance  $r_e$  of the  $X^4\Delta$  electronic state of FeH. Our results are presented in Table 1 together with the previous values obtained by Tanaka, Sekiya, & Yoshimine (2001) and by Langhoff & Bauschlicher (1990).

Table 1. Energy\* values near the equilibrium distance† of  $X^4\Delta$  of FeH

States	Present work		Langhoff <i>et al.</i>		Tanaka <i>et al.</i>		Experiment	
	$E$	$r_e$	$E$	$r_e$	$E$	$r_e$	$E$	$r_e$
$X^4\Delta$ .....	0	2.964	0	3.001	0	3.016	0	3.002
$A^4\Pi$ .....	1309	2.917	1200	2.934	2010	2.933	930	...
$a^6\Delta$ .....	372	3.190	1290	3.199	2080	3.235	1970	3.34
$b^6\Pi$ .....	2183	3.181	3244	3.197	3310	3.207	4010	...
$c^6\Sigma^+$ .....	4249	3.203	3694	3.201	4600	3.190	4870	...

\*Adiabatic term energy in  $\text{cm}^{-1}$

†Equilibrium distance in  $a_0$

### 4. Conclusion

Lines and photodissociation cross sections have been calculated for MgH using a full theoretical treatment, improving the previous extrapolated results. Progress has been made in the determination of *ab initio* potential energy surfaces for LiCl and FeH, in order to calculate for the first time complete absorption spectra of both molecules.

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